

THE TWO - DIMENSIONAL ATTRACTIVE HUBBARD MODEL: HIGHLY NON-LINEAR SUPERCONDUCTIVITY WITH SUM RULES.

J.J. Rodríguez-Núñez

*Departamento de Física, Universidade Federal de Santa Maria, CCNE, 97105 - 900 Santa Maria/RS, Brazil.
e-m: jjrn@mfis.ccne.ufsm.br*

C.E. Cordeiro and A. Delfino

*Instituto de Física, Universidade Federal Fluminense, Av. Litorânea S/N, Boa Viagem, 24210-340 Niterói/RJ, Brazil.
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We use the moment approach of Nolting (exact sum rules) (Z. Physik **255**, 25 (1972)) for the attractive Hubbard model in the superconducting phase. Our diagonal and off - diagonal spectral functions are constructed and evaluated with the sum rules. They reduce to the *BCS* limit for weak interaction. However, the presence of correlations modify the *BCS* picture dramatically. For example, due to the presence of correlations we have postulated a three - pole ansatz for the diagonal Green function, $G(\vec{k}, \omega)$, while the off - diagonal one, $B(\vec{k}, \omega)$, is supposed to have two poles. In the paper we present results for the three spectral weights of the diagonal Green function, $\alpha_j(\vec{k})$, $j = 1, 2, 3$. Our results compare reasonably well with more elaborated auto - consistent highly non - linear equations (double fluctuation calculations in the T - Matrix approach of one of the authors). Then, the physical picture which emerges is that the lower Hubbard band is split due to the superconducting gap and the upper Hubbard band remains mostly unmodified.

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I. INTRODUCTION

The study of correlations has been renewed again by the the discovery of high T_c superconducting oxide materials (HTSC), [1] since that these materials exhibit a short coherence length, ξ , and a very large penetration depth, λ , which become them almost extreme type-II superconductors, i.e. $\kappa \equiv \frac{\lambda}{\xi} \gg 1$.

In order to study the effect of correlations we will use the on-site attractive Hubbard Hamiltonian put forward by Micnas et al [2] as a phenomenological model for describing the HTSC. Previous authors have used this model to study the bismuthate superconductors. [3] Denteneer et al [4] recognize that if the phase diagram of the Hubbard model were fully understood, it might form the basis of understanding correlated electrons as much as the Ising model did for understanding critical phenomena. More recently, Schneider et al [5] have applied this model to explain universal properties of several families of these compounds, like the relation between transition temperature, magnetic penetration depth and gap, at zero temperature.

In this paper, we will use the exact relations of Nolting [6] for the one-particle diagonal spectral function together with the exact relations for the one-particle off-diagonal spectral function, i.e., the anomalous Green's function, to study systems with broken symmetry. [7]

The model we study is the following

$$H = -t \sum_{\langle i,j \rangle \sigma} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} - \mu \sum_{i\sigma} n_{i\sigma} \quad , \quad (1)$$

where $c_{i\sigma}^\dagger$ ($c_{i\sigma}$) are creation (annihilation) electron operators with spin σ . $n_{i\sigma} \equiv c_{i\sigma}^\dagger c_{i\sigma}$, t is a hopping matrix element between the nearest sites (n.n.) i and j , and U is the onsite interaction. μ is the chemical potential and we work in the grand canonical ensemble. In the present study we consider an attractive interaction, $U \equiv -|U| < 0$. The Hamiltonian of Eq. (1) has been studied in detail by Micnas et al [2]. Nolting [6] and Kalashnikov and Fradkin [7] have derived exact relations for the one-particle spectral functions which are given in Ref. [8].

We postulate for the diagonal spectral function, $A(\vec{k}, \omega)$, the following ansatz

$$A(\mathbf{k}, \omega) \equiv \alpha_1(\vec{k})\delta(\omega - E_{\vec{k}}) + \alpha_2(\vec{k})\delta(\omega + E_{\vec{k}}) + \alpha_3(\vec{k})\delta(\omega - \Omega_{\vec{k}}) \quad (2)$$

and the off-diagonal spectral function, $B(\vec{k}, \omega)$, is supposed to have two peaks (*BCS*-like), as follows

$$B(\vec{k}, \omega) \equiv \sqrt{\alpha_1(\vec{k})\alpha_2(\vec{k})} [\delta(\omega - E_{\vec{k}}) - \delta(\omega + E_{\vec{k}})] \quad , \quad \Omega_1(\vec{k}) = E_{\vec{k}} \quad , \quad \Omega_2(\vec{k}) = -E_{\vec{k}} \quad (3)$$

Our ansatz is based on the assumption that the diagonal spectral function is modified by the presence of correlations (we define correlations when we have the regime $U/W \approx 1$, where $W = 8t$ is the bandwidth in two dimensions). This assumption has been numerically checked to be correct in Ref. [9] where the authors have obtained three bands for the diagonal spectral function and two bands for the off-diagonal spectral function after performing the analytical continuation. In Eq. (2), the first two poles represent the behavior around the chemical potential and the third pole is due to the influence of the upper Hubbard band, which in the case of the atomic limit is the upper Hubbard band or the band of single occupied states. The lower band, now split in two, is the band of double occupied states for the case of almost atomic limit. Please, see reference [10], where the attractive Hubbard model has been studied in the normal phase with two different methods: T -Matrix and moments.

The order parameter, $\Delta_o(T)$, and the chemical potential (fixed electron density), μ , are calculated from the following equations:

$$\Delta_o(T) = \frac{1}{N} \sum_{\vec{k}} \int_{-\infty}^{+\infty} \frac{B(\vec{k}, \omega)}{e^{\beta\omega} + 1} \quad ; \quad \rho = \frac{1}{N} \sum_{\vec{k}} \int_{-\infty}^{+\infty} \frac{A(\vec{k}, \omega)}{e^{\beta\omega} + 1} \quad . \quad (4)$$

For example, the quasi-particle energy, $E_{\vec{k}}$, has a gap. As it was discussed in Ref. [8], the gap is expressed in terms of the order parameter as

$$\Delta(T, \vec{k}) = \Delta_0(T) \frac{2E_{\vec{k}}}{E_{\vec{k}} + a_1(\vec{k})} \quad , \quad (5)$$

concluding from Eq. (5) that our gap equation, which is a manifestation of singularities in the density of states, is \vec{k} -dependent. Going back to our local Hamiltonian (see Eq. (1)), which in reciprocal space is a constant, then at the mean field level we should obtain a *pure s-wave*, while going beyond mean field approximation we have been able to derive a \vec{k} -dependent gap. In our case, by including correlations, i.e., the selection rules for a_2 and a_3 (See Ref. [8] for more details) we have been able to modify the BCS results, from pure s-wave to a wave vector dependent energy gap. Let us point out that in the attractive Hubbard model we always find *s*-type wave symmetry as it has conclusively shown in Ref. [11] in the Hubbard-I approximation for both the diagonal and the off-diagonal one-particle Green functions.

We would like to call the reader's attention that our Ansatz is based on the assumption that the role of correlations is mainly taken into account in the diagonal one-particle spectral function. This implies that the off-diagonal order parameter has been taken at the BCS level, i.e., to $M^{(1)}(\mathbf{k})$. In a previous work, [12] it is found that both the diagonal and off-diagonal spectral functions have four peaks, symmetric in pairs, for $U/t = -4$. However, when we have included double fluctuations, i.e., fluctuations in both the diagonal and off-diagonal self-energies as in Ref. [9], we have three resolved peaks for $A(\vec{k}, \omega)$ and two well resolved peaks for $B(\vec{k}, \omega)$. So, Ref. [9] has motivated us to adopt three and two peaks for $A(\vec{k}, \omega)$ and $B(\vec{k}, \omega)$, respectively, for $U/t = -4.0$. We have restricted ourselves to wavevectors close to the chemical potential. If we want to consider two other peaks for the off-diagonal spectral function we have to include more moments, which is beyond the present work. Also, we have neglected life-time effects in Eqs. (2-3), which would require to approach the phase transition with damping in the self-energy as it has been done in Ref. [13].

The equations we have to solve are the following

$$\frac{1}{U} = -\frac{1}{N} \sum_{\mathbf{k}} \frac{\tanh(\frac{\beta E_{\mathbf{k}}}{2})}{2E_{\mathbf{k}}} \quad (6)$$

$$\rho = \frac{1}{N} \sum_{\mathbf{k}} \left[\alpha_1(\mathbf{k})f(E_{\mathbf{k}}) + \alpha_2(\mathbf{k})f(-E_{\mathbf{k}}) + \frac{a_1(\mathbf{k}) - \Omega_1(\mathbf{k})}{\Omega_2(\mathbf{k}) - \Omega_1(\mathbf{k})} f(\Omega_{\mathbf{k}}) \right] \quad (7)$$

In Fig. 1 we show the dependence of the diagonal spectral weights, $\alpha_j(\vec{k})$, $j=1,2,3$ along the diagonal of the Brillouin zone. We can appreciate that the area of the spectral function is equal to one ($\alpha_1 + \alpha_2 + \alpha_3 = 1$) by construction. We have taken $U/t = -4.0$, $\rho = 0.1$ and $T/t = 0.01$. After self-consistency of our highly non-linear equations we obtain $\mu/t = -4.19$, $B/t = 1.664$ and $\Delta_0(T) = 0.52$. It is worth mention that $\mu < -4t$ which indicates that we are in the low density regime (Bose - Einstein limit). In Fig. 2 we have the diagonal spectral weights along the k_x -axis ($\vec{k} = (k, 0)$). What we observe is a strong variation of the $\alpha_j(\vec{k})$ with direction. In Fig. 3 we have the \vec{k} -dependence of $\gamma_j(\vec{k})$, $j =$

1,2 along the two directions as previously discussed in Figures 1 and 2. These $\gamma_j(\vec{k})$'s are defined by Eq. (19) in Ref. [8]. They are highly \vec{k} -dependent. The meaning of these variables is that they represent corrections to the diagonal sum rules ($a_2(\vec{k})$ and $a_3(\vec{k})$). As we have said in Ref. [8] these corrections are important, i.e., of the order of 20 - 25 higher corrections on the order parameter (or equivalently, $\gamma_j(\vec{k})$'s). For $T \approx T_c$ these corrections are not important, though.

By using the moment approach in the presence of off-diagonal long range order, i.e., $\Delta_o(T) \neq 0$, to the negative Hubbard model, we have worked out the superconducting phase calculated with the use of moments (exact sum rules for both the diagonal and off-diagonal spectral densities) with three and two and two peaks, respectively. The physical meaning of each of these peaks has been discussed. This assumption is equivalent to solve the diagonal spectral weights in powers of the order parameter square. At the same time, we have seen that the effect of the third band is to renormalize the order parameter producing an energy gap which is \vec{k} -dependent. In consequence, in our approach the order parameter, $\Delta_o(T)$, and the energy gap, $\Delta(T, \vec{k})$ are not the same. We would like to end by saying that there are strictly mean - field calculations (even if they go beyond Hartree - Fock) as the ones done by Martín - Rodero and Flores [14] and Kuchiev and Sushkov [15]. Our approach presented here is able to capture the double fluctuation calculation of Ref. [9]. This clearly indicates that we are beyond a simple *BCS* calculations.

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Figures

Figure 1. The spectral weights, $\alpha_j(\vec{k})$, $j = 1, 2, 3$ along the diagonal of the Brillouin zone. The first diagonal sum rule is satisfied. $U/t = -4.0$, $\rho = 0.1$ and $T/t = 0.01$.

Figure 2. The spectral weights, $\alpha_j(\vec{k})$, $j = 1, 2, 3$ along the k_x direction of the Brillouin zone. Same parameters as in Figure 1.

Figure 3. $\gamma_j(\vec{k})$, $j = 1, 2, 3$ along the two directions discussed in Figures 1 and 2. Same parameters as before.





